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Weak and strong coupling of surface polaron at the contact of two polar crystals

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Abstract : Weak and strong couplings of surface polaron in the framework of variational method were studied theoretically. We have obtained a result which shows that it is possible to reinforce the polaron effect in the low dimensional system

Keywords Fröhlich-Pekar Hamiltonian, weak coupling, strong coupling, surface polaron, interface of two polar crystals

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1. Introduction

The problem of surface polaron is studied in [1-4], a weak coupling of surface polaron in ionic crystal is studied in [5]. A theory of surface polaron states at contact of two polar media for a weak coupling on the basis of the generalized Hamiltonian of Fröhlich-Pekar type is developed in [6]. On the basis of polaron approach, the potential $U_T(Z)$ which is caused by surface and bulk optical vibrations, is obtained. For large value of Z (Z is the distance of charge carrier at interface) in comparison with polaron radius R_v, $R_v = (\hbar / 2m^* \omega)^{1/2}$, $U_T(Z)$ passes into electrostatic imaging potential. However, in the region of contact, $U_T(Z)$ is a non-monotonic function of Z. For example, at contact of non-polar crystal with vacuum $\varepsilon_2 = 1$, for electron which exists in crystal at $\varepsilon_1 < 2.2$, interaction with interface has a repulsion character. At $\varepsilon_1 < 2.2$, the potential $U_T(Z)$ in the range $Z \sim R_v$ is maximum which separates the repulsion region at greater value of Z from the attraction region at small value of Z [7]. Connection of polaron state with surface at $Z \sim R_v$ will appear, when $U_T(Z)$ passes a low free bulk optical phonon level.

$$U_T(Z) < \alpha_v \hbar \omega_0, \tag{1}$$

where α_v is the electron-phonon interaction constant ; ω_0 is the frequency of bulk longitudinal optical phonons. Condition of finding surface state (1) is considered more general than the condition $\varepsilon_2 > \varepsilon_1$ which determines the attraction character of the potential U_{ie}. In Ref. [6], the energy of surface polaron bond at the contact of two polar crystals, when the motion of an electron in the direction of Z is slow in comparison with the motion in the direction of the surface, is obtained. We will study the problem of surface polaron, when this condition is not satisfied. In the present work, surface polaron states in the framework of variational method for an arbitrary bond, on the basis of generalization of Hamiltonian of Fröhlich-Pekar type are studied theoretically.

2. Hamiltonian and variational energy

Let us consider the interface between two polar crystals, the first occupying a half space $Z < 0$ ($K = 2$), and the second occupying a half space $Z \geq 0$ ($K = 1$), both having the dielectric permittivities $\varepsilon_{02}, \varepsilon_2$ and $\varepsilon_{01}, \varepsilon_1$ respectively ($\varepsilon_{n0}, \varepsilon_n$ are static and high-frequency dielectric permeability of crystals). Let us assume that an electron exists in the conduction band of the second crystal and interact with surface and bulk optical phonons.

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The Hamiltonian of the system under investigation is

$$\hat{H} = \frac{\hat{P}_{\perp}^2}{2m_{\perp}^*} + \frac{\hat{P}_{\parallel}^2}{2m_{\parallel}^*} + \frac{e^2(\varepsilon_1 - \varepsilon_2)}{4Z\varepsilon_1(\varepsilon_1+\varepsilon_2)} + \sum_{\eta, j=1,2} \hbar\Omega_{sj}\, \hat{b}_{\eta j}^+ \hat{b}_{\eta j}$$

$$+\sum_{Q} \hbar\omega_0 \hat{b}_Q^+ \hat{b}_Q + \sum_{\eta, j} V_{sj} e^{i\eta\rho} e^{-\eta z}\left(\hat{b}_{-\eta j}^+ + \hat{b}_{\eta j}\right)$$

$$+\sum_{Q} V_B\left(e^{iq_z Z} - e^{-\eta Z}\right) e^{i\eta\cdot\rho}\left(\hat{b}_{-Q}^+ + \hat{b}_Q\right) + V_B(Z), \tag{2}$$

where

$$^2 = \frac{2\pi\alpha_{sj}\,(\hbar\Omega_j)^2 R_{sj}}{L_x L_y \eta}, \quad R_{sj} = \left(\frac{\hbar}{2m^*\Omega_j}\right), \tag{3}$$

$$|V_B|^2 = \frac{4\pi\alpha_v\,(\hbar\omega_0)^2 R_v}{L_x L_y L_z Q^2}, \quad R_v = \left(\frac{\hbar}{2m^*\omega_0}\right)^{1/2}, \tag{4}$$

where α_{sj}, α_v are defined in Ref. [6].

$$V_B(Z) = \begin{matrix} \infty, & Z<0 \\ 0, & Z \ge 0 \end{matrix} \tag{5}$$

is the potential barrier in the interface.

From Ref. [8], by introducing the first transformation operator S_1 on the Hamiltonian (2), where

$$\hat{S}_1 = \exp\left\{-ia\left(\sum_{\eta, j=1,2} (\eta\cdot\rho)\hat{b}_{\eta j}^+ \hat{b}_{\eta j} + \sum_{Q} (Q\cdot\rho)\hat{b}_Q^+ b_Q\right)\right\}, \tag{6}$$

where a-is the parameter which determines the electron-phonon coupling forces.

$a = 1$, corresponds to weak and intermediate coupling.

$a = 0$, corresponds to strong coupling.

After that the second transformation operator S_2 is performed on the resulting Hamiltonian. The result is averaged over the phonon vacuum states $|0\rangle_v, |0\rangle_s$:

$$\hat{S}_1 = \exp\left\{\sum_{\eta, j}\left(\hat{b}_{\eta j}^+ f_{\eta j} - \hat{b}_{\eta j} f_{\eta j}^*\right) + \sum\left(\hat{b}_Q^+ f_Q - \hat{b}_Q f_Q^*\right)\right\} \times$$

$$\psi(Z)\,|0\rangle_v\,|0\rangle_{sj}. \tag{7}$$

Here, $\psi(Z)$ is the variational wave function which describes the motion of electron in the direction Z axis. In the infinite potential barrier approximation, $\psi(Z)$ takes the form

$$\psi(Z) = 2\beta^{3/2} e^{-\beta z}, \tag{8}$$

β is a variational parameter, $f_{\eta j}, f_{\eta j}^*, f_Q, f_Q^*$ are variational parameters to be determined later.

Then the variational ground state energy is given by

$$E_0(\beta, \lambda, a) = \frac{\hbar\lambda}{2}(1-a)^2 + \frac{\hbar^2\beta^2}{2m_Z^*} + \frac{e^2(\varepsilon_1 - \varepsilon_2)\beta}{4\varepsilon_1(\varepsilon_1+\varepsilon_2)}$$

$$-\sum_{j=1,2} \frac{|V_{sj}|^2}{\hbar\Omega_{sj}} J_1(\beta, \lambda, a) - \frac{e^2(\varepsilon_{1\infty} - \varepsilon_1)\beta}{\pi\varepsilon_{1\infty}\varepsilon_1} J_2(\beta, \lambda, a), \tag{9}$$

where

$$J_1 = \int_0^{\infty} d\eta\, \exp\left[\frac{-\hbar^2}{2m_{\perp}^*\lambda}(1-a^2)\eta^2\right]\left(1+\frac{\eta}{2\beta}\right)^{-}$$

$$\left(1+a^2 R_{sj}\eta^2\right)^{-1}, \tag{10a}$$

$$J_2 = \int^{\infty} d\eta\, \exp\left[\frac{-\hbar^2}{2m_{\perp}^*\lambda}(1-a^2)\eta^2\right] \int^{\infty} dq_z\left[1 + a^2 R_v^{\frac{1}{2}}(\eta^2 + q_z^2)\right]$$

$$\times\left(\eta^2 + q_z^2\right)^{-1} \times \left\{\left(1+\frac{q_z^2}{4\beta^2}\right) + \left(1+\frac{\eta}{2\beta}\right) - 2\left(1-3\frac{q_z^2}{4\beta^2}\right)\right.$$

$$\left.\times\left(1+\frac{\eta}{2\beta}\right)\left(1+\frac{q_z^2}{4\beta^2}\right)\right\}. \tag{10b}$$

It is very difficult to put eq. (9) in the analytic form. But it is possible to obtain the numerical minimization in the case of plane polaron at the contact of two polar crystals.

From the variational condition

$$\frac{\partial E_0}{\partial f_Q^*} = \frac{\partial E_0}{\partial f_{\eta j}^*} = 0, \tag{11}$$

one obtains

$$f_{\eta j} = \frac{-V_{sj}^*[1+\eta/(2\beta)]\exp\left[-\hbar(1-a^2)\eta^2/(4m_{\perp}^*\lambda)\right]}{\hbar\Omega_{sj} + a^2\hbar^2\eta^2/(2m_{\perp}^*)}, \tag{12a}$$

$$f_Q = \frac{-V_B^*\left([1-iq_z/(2\beta)]^{-3} - [1+\eta/(2\beta)]\right)^3}{\hbar\omega_0 + a^2\hbar^2 Q^2}$$

$$\frac{\exp\left[-\hbar(1-a^2)\eta^2/(2m_{\perp}^*\lambda)\right]}{/(2m_{\perp}^*)}, \tag{12b}$$

where

$$V_{sj}^{*} = V_{sj}\langle\psi(Z)|\, e^{-\eta Z}\,|\psi(Z)\rangle, \tag{13a}$$

$$V_{B}^{*} = V_{B}\langle\psi(Z)|\, e^{-iq_{\iota}Z} - e^{-\eta Z}\,|\psi(Z)\rangle. \tag{13b}$$

3. Plane polaron in the contact of two polar crystal

In this section, the plane polaron (Z = 0) in the contact of two polar crystals is studied. This case can be realized for polarization charge carrier, when the wave vector diminishes in the direction of Z and stays less than polaron radius.

Eq. (9) passes to the limit β obtain

$$\bar{E}_0(\lambda,a) = \tilde{\lambda}(1-a)^2 - \sum_{j=1,2}\frac{|V_{sj}|^2\lambda^{1/2}}{\hbar^2\Omega_{s1}\Omega_{sj}} J_{1j}(\tilde{\lambda},a), \tag{14}$$

here

$$J_{1j}(\tilde{\lambda},a) = \int^{\infty} e^{-x^2}\; 1 + \frac{a\bar{\lambda}x^2}{(1-a)\gamma}\; dx,$$

where

$$\gamma = \frac{\Omega_{sj}}{\Omega_{s}},\ \tilde{\lambda} = \frac{\lambda}{\Omega_{s1}},\ \tilde{E}_0(\tilde{\lambda},a) = \frac{\bar{E}_0(\lambda,a)}{\hbar\Omega_{s1}}.$$

By entering the new variable

$$y = \frac{1-a}{a\sqrt{\lambda}}, \tag{15}$$

and integrating eq. (14) obtain

$$E_0(\lambda,y) = \frac{\tilde{\lambda}}{2\left[1+1/\left(\sqrt{\tilde{\lambda}}\,y\right)\right]^2} - \frac{\pi}{2}\left\{\alpha_{s1}\left(\sqrt{\tilde{\lambda}}y+1\right)e^{y^2}\left[1-\phi(y)\right]\right.$$

$$\left. {}_{s2}\,\gamma\left(\sqrt{\tilde{\lambda}}y+1\right)e^{\gamma y^2}\left[1-\phi(\sqrt{8}y)\right]\right\}, \tag{16}$$

where $\phi(x)$ is the probability function.

In the limit of a weak coupling $a = 1$, $\alpha_s << 1$, and minimize eq. (16) on y and $\tilde{\lambda}$ obtain

$$\bar{E}_0 = -\frac{\pi}{2}(\alpha_{s1}+\gamma\alpha_{s2}) - \frac{\pi^2}{512}\frac{(\alpha_{s1}+\gamma\alpha_{s2})^4}{\left(\alpha_{s1}+\gamma^{3/2}\alpha_{s2}\right)^2}. \tag{17}$$

In the limit of strong coupling $a = 0$, from eq. (16) obtain

$$\bar{E}_0 = -\frac{\pi}{8}\left(\alpha_{s1}+\sqrt{\gamma}\alpha_{s2}\right)^2 - \frac{\left(\alpha_{s1}+\sqrt{\gamma}\alpha_{s2}\right)}{2\left(\alpha_{s1}+\alpha_{s2}/\sqrt{\gamma}\right)}. \tag{18}$$

If the result we have obtained are compared with the known result for plane system in the case of constant polar crystal with non-polar crystal, then one of the two surface modes $(\Omega_{s1},\Omega_{s2})$ remains one mode only $(\alpha_{s2} = 0)$. Therefore

a) Weak coupling

$$\bar{E}_0 \cong -\frac{\pi}{2}\alpha_s - \frac{\pi^2}{512}\alpha_s^2 = -\frac{\pi}{2}\alpha_s - 0.0606\alpha_s^2. \tag{19a}$$

b) Strong coupling

$$\bar{E}_0 \cong -\frac{\pi}{8}\alpha_s^2 = -0.3028\alpha_s^2. \tag{19b}$$

In these limits Ref. [9] gives the following results

$$E_0 = -\frac{\pi}{2}\alpha_s - 0.064\,\alpha_s^2, \quad \text{for a weak coupling;} \tag{20a}$$

$$\bar{E}_0 = -0.4047\,\alpha_s^2, \quad \text{for a strong coupling.} \tag{20a}$$

By comparing the results obtained in this study with those obtained in [9], it follows that the best agreement has been obtained in the region of weak coupling. It is noted that in the limit of strong electron-phonon coupling, the contribution caused by the surface modes in energy, is not additive. This result shows that it is possible to reinforce the polaron effect in the low dimensional system.

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